Electrodynamics of a Clean Vortex Lattice

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We report on a microscopic evaluation of electrodynamic response for the vortex lattice state of a model s-wave superconductor. Our calculation accounts self-consistently for both quasiparticle and order parameter response and establishes the collective nature of linear response in the clean limit. We discuss the effects of homogeneous and inhomogeneous pinning on the optical conductivity and the penetration depth, and comment on the relationship between macroscopic and local penetration depths. We find unexpected relationships between pinning arrangements and conductivity due to the strongly non-local response.

74.25.Gz,74.60.-w,74.60.Ge,74.25.Nf

The study of vortex electrodynamics in type II superconductors has been ongoing for over 30 years [1]. Due to the complexity of the problem, however, the theory of vortex electrodynamics remains incomplete. For a system with perfect translational invariance, it can be shown rigorously that the long-wavelength response consists only of a resonance at the cyclotron frequency [2], so that there is no signature of superconductivity in the a.c. conductivity. In real systems the response is complicated by broken translational symmetries associated with disorder, pinning defects and even the underlying atomic lattice. Relatively few rigorous results exist for the general case. One regime which has been extensively studied is the the dirty limit of vortex core sizes ξ much larger than quasiparticle mean-free-paths ℓ. In this case, the response is approximately local and the Bardeen-Stephen [3,4] isolated vortex model provides a useful picture. Even in the dirty limit, vortex-vortex interactions play an important role in the electrodynamics except at fields very close to H_{c1} and microscopic models rapidly become intractable. Instead, one typically interprets experiments at sub-THz frequencies in terms of simpler phenomenological hydrodynamic models [5,6,11], in which the mixed state is characterized by vortex pinning, viscosity, and interaction parameters.

No comparable phenomenology exists for the clean-limit vortex lattice, for which ℓ is larger than ξ or even larger than the distance between vortices. In this case the details of disorder within a particular vortex core [7] become important and nonlocal response can make the connection between single-vortex models [8] and the dense vortex systems tenuous. Interest in the clean limit has grown in recent years with the advent of clean single crystals of type II low (s-wave) and high (d-wave) T_c materials. In particular, the extent to which in-field optical conductivity measurements can be used as a probe of fundamental properties of high T_c materials is a subject of great interest [9,10]. Existing experimental work is confusing and possibly contradictory. Resonances have been observed in thin films of $YBa_2Cu_3O_{7-\delta}$ (YBCO) and were interpreted as being due to vortex core transitions [12], the clean-limit manifestation of vortex mo-

tion [16]. Other, possibly related, resonances observed in $Bi_2Sr_2CaCu_2O_8$ (BSCCO) [13] were interpreted as being due to collective vortex motion. In contrast, recent experiments [9] in thin films of BSCCO were convincingly interpreted in terms of a continuum of extended quasiparticle states, ignoring vortex motion. Finally, infrared measurements of YBCO crystals have failed to find any appreciable field-dependence to the conductivity [14] at all!

Much of the theoretical work on electrodynamics in the clean limit has been based on one of two extreme pictures; in the first [15] quasiparticle states of the vortex lattice respond directly to the perturbing electromagnetic field without any order parameter response, while in the second [7,16] it is the vortices that move, usually rigidly, and indirectly disturb the quasiparticle equilibrium. Another stimulating approach uses a phenomenological composite model to interpret the multiple resonances and magnetooptical activity seen in experiment [17]. The difficulty which arises in any serious calculation, however, is that quasiparticles and vortices are not separate entities. A time-dependent order parameter, for example one arising from vortex motion, creates a time-dependent potential for the quasiparticle states from which the order parameter is in turn constructed.

In this Letter we report on a microscopic calculation which treats the order parameter and the quasiparticles on equal footing [18], and which naturally captures the nonlocal nature of clean-limit vortex electrodynamics. In this case, the appropriate language is not that of quasiparticles interacting with moving vortices, but is instead that of collective modes. The approach is microscopic and proceeds in three steps. First we calculate a self-consistent solution for the equilibrium vortex lattice using the Bogoliubov-deGennes (BdG) equations. Second we evaluate the linear response of normal and anomolous blocks of the one-particle density matrix to a perturbing electromagnetic (EM) field, accounting for vortex motion and distortion self-consistently. Third, we use the density matrix to find the induced current, and therefore the conductivity. Since this is a linear response calculation it addresses external fields which produce a vortex

displacement that is small compared to the coherence length. Because the equations are solved in real space, it is a trivial matter to incorporate disorder or other forms of broken translational invariance.

There are two important energy scales in our discussion. The first is the cyclotron energy $\hbar\omega_c$, which is the resonant frequency of a translationally invariant superconducting system [2]. The second is the quasiparticle absorption energy $\hbar\omega_{qp} \sim \Delta^2/W \sim \hbar\omega_c(H_{c2}/H)$ [19], where Δ is the s-wave gap, W is the metal band-width, and H is the field-strength. This is the predicted energy of allowed transitions between vortex core states in non-self-consistent calculations which ignore vortex motion [15]. Note that the cyclotron frequency drops below the quasiparticle bound state transition energy as the external field drops below H_{c2}. Before turning to a discussion of our results, we briefly outline the formulation of vortex-lattice equilibrium state and response-function theory on which they are based.

We have obtained self-consistent solutions of mean-field equations for equilibrium and linearly perturbed states of two-dimensional generalized Hubbard model Hamiltonians. We use a Nambu vector notation, defining $\mathbf{C} = (c_1, c_2, \ldots, c_{2N})$ where, $c_i = c_{i\uparrow}$, $c_{i+N} = c_{i\downarrow}^\dagger$, $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are creation and annihilation operators for site i and spin σ, and N is the number of lattice sites. The mean field hamiltonian can then be written as $\mathcal{H}^{MF} = \mathbf{C}^\dagger\mathbf{H}^{\mathbf{BG}}\mathbf{C}$ where $\mathbf{H}^{\mathbf{BG}}$ is the $2N \times 2N$ Bogoliubov-de Gennes matrix:

$$\mathbf{H}^{\mathbf{BG}} = \begin{bmatrix} \tilde{\epsilon} - \mu\mathbf{1} & \mathbf{\Delta^0} \\ \mathbf{\Delta^{0\dagger}} & -\tilde{\epsilon}^* + \mu\mathbf{1} \end{bmatrix}. \qquad (1)$$

Here $\tilde{\epsilon}$, and $\mathbf{\Delta}$ are $N \times N$ matrices and μ is the chemical potential. The one-body matrix elements, $\tilde{\epsilon}_{ji}$ can be used to model intersite hopping, and diagonal or off-diagonal disorder. The magnetic field, which we take to be uniform, is accounted for by multiplying all one-particle matrix elements by Landau gauge phase factors; $\tilde{\epsilon}_{ji} = \epsilon_{ji}\exp(i\alpha Y_i(X_j - X_i))$ where (X_i, Y_i) is the location of the i-th lattice site and $\alpha = eB/\hbar c$. $\Delta_{ij} = V_{ij}\langle c_{j\downarrow}c_{i\uparrow}\rangle$ where V_{ij} is the Hubbard model interaction strength between sites i and j and the angle brackets denote a consistently determined thermal average. We enforce periodicity [20,21] in a supercell containing an even-integer number of vortices, typically two. The mean-field Hamiltonian can be written in the diagonal form, $\mathcal{H}^{MF} = \sum_n E_n \gamma_n^\dagger \gamma_n$ where E_n is an eigenvalue of $\mathbf{H}^{\mathbf{BG}}$, $\gamma_n = \sum_i U_{n,i}^* c_i$ is a fermionic quasiparticle annihilation operator, and $\mathbf{U}$ specifies the unitary transformation that diagonalizes $\mathbf{H}^{\mathbf{BG}}$. ($\mathbf{U}^\dagger\mathbf{H}^{\mathbf{BG}}\mathbf{U} = \mathbf{E}$ where $\mathbf{E}$ is the diagonal matrix with elements E_n.) The equilibrium density matrix is $\rho^0 = \exp(-\beta\mathcal{H})/Z$ with $Z = \mathrm{Tr}\,\exp(-\beta\mathcal{H})$, $\beta = 1/k_B T$, and the order parameter equation is

$$\Delta_{ij}^0 = V_{ij}[\mathbf{U}\rho^0\mathbf{U}^\dagger]_{ij+N}, \qquad (2)$$

Note that in our notation, half of the quasiparticles states are occupied in the ground state. Eq. [2] is the vortex-lattice state analog of the simple Meissner state gap equation and can be solved iteratively.

The linear response of the density matrix at frequency ω is given by the following familiar expression:

$$\delta\rho_{n',n}(\omega) = \frac{f(E_n) - f(E_{n'})}{\hbar\omega - E_{n'} + E_n + i\eta}[\mathbf{U}^\dagger\delta\mathbf{H}^{\mathbf{BG}}\mathbf{U}]_{n',n} \quad (3)$$

$\delta\mathbf{H}^{\mathbf{BG}}$ has a contribution ($\delta\tilde{\epsilon}$) in its diagonal blocks, which describes the coupling of a weak a.c. electric field to the system [21,22], and a contribution in the off-diagonal blocks,

$$\delta\Delta_{ij}'(\omega) = V_{ij}[\mathbf{U}\delta\rho(\omega)\mathbf{U}^\dagger]_{ij+N}, \qquad (4)$$

which describes the self-consistent response of the order parameter. In non-self-consistent calculations the latter contribution is neglected. Multiplying, Eq. (3) by the energy denominantor, leads to a set of linear equations for $\delta\rho_{n'n}$ which can be solved by inverting a symplectic [21] matrix that is singular when $\hbar\omega$ equals a collective excitation energy of the system. Since

$$\delta O = \sum_{n',n}\langle n'|O|n\rangle\delta\rho_{n,n'}, \qquad (5)$$

we can calculate the linear response of any observable to the perturbing a.c. field. The complex optical conductivity tensor $\sigma_{\mu\nu}(\omega)$ is defined by $\delta J_\mu = \sum_\nu \sigma_{\mu\nu}(\omega)E_\nu(\omega)$, where $\mathbf{J}$ is the current operator and $\mathbf{E}(\omega)$ is the a.c. electric field. Here we report results for an on-site attractive pairing model ($V_{ij} = -V_0\delta_{i,j}$) which leads to s-wave superconductivity. It is convenient to compare normal and superconducting state response by adjusting the strength of the pairing interaction, rather than field strength or temperature. The chemical potential is chosen near the bottom of the band where the dispersion is nearly parabolic.

Resonances in the conductivity are determined by the pole structure of the nonequilibrium density matrix $\delta\rho(\omega)$, shown in Fig. 1. While $\delta\rho(\omega)$ has a complicated spectrum, only a small subset of all possible resonances are excited by a long wavelength EM field, and the remaining resonances are optically silent. In fact, in the absence of pinning and disorder there is essentially only one optically active resonance, which occurs at a frequency ω_0 near ω_c, and well below ω_{qp}, as shown in the top panel of Fig. 2 where the real part of the circularly polarized conductivity [$\sigma^+(\omega) \equiv \sigma_{xx}(\omega) + i\sigma_{xy}(\omega)$] is plotted. We stress that the absence of a peak in the conductivity at ω_{qp} is not a product of changes in optical selection rules brought about by vortex motion, but rather reflects the absence of a pole in $\delta\rho(\omega)$ at that frequency, as shown explicitly in Figs. 1 (a) and (b). This underscores the collective nature of the excitation spectrum of the vortex lattice.

In the absence of extrinsic pinning, the small frequency shift $\omega_0 - \omega_c$ of the response is a result of broken translational invariance by the lattice. In general, we expect
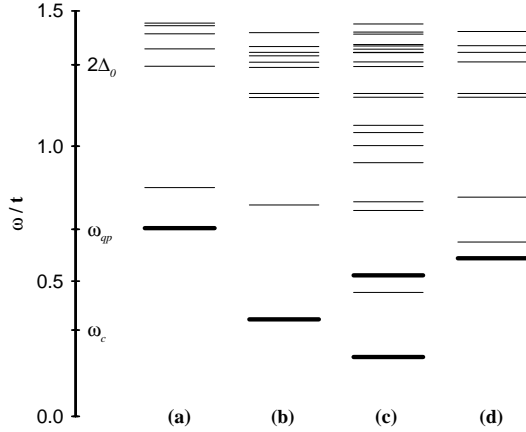
FIG. 1. Spectrum of the nonequilibrium density matrix $\delta\rho(\omega)$ at $T = 0$. (a) Non-self-consistent calculation, (b) Self-consistent calculation, (c) With single pinning center per unit cell, (d) With two pinning centers per unit cell. Optically active resonances with a large spectral weight are indicated by thick solid lines. The weaker spectral weights are smaller by at least one order of magnitude. The resonant frequencies in (a) correspond to quasiparticle energy differences. Results are for a magnetic unit cell containing two vortices and 32 lattice sites.

FIG. 2. Real part of the electron-active circularly polarized conductivity of vortex lattice states. *Top:* V_0' has the same value at all vortex cores. Results of a non-self-consistent calculation are also shown. *Bottom left:* Every second vortex core is pinned. *Bottom right:* Effect of pinning on the penetration depth. Open bars are for inhomogeneous pinning. Conductivity is measured in units of tf_{tot} where t is the nearest neighbour hopping energy.

vortex motion to be strongly influenced by the atomic lattice when the coherence length is comparable to the atomic lattice spacing, a situation which may in fact be realised in BSCCO [23]. The effects of including homogeneous extrinsic pinning are also shown in the top panel of Fig. 2. Pinning is modelled here by reducing the pairing interaction V_0 to a smaller value V_0' at each vortex core center, a change which has no effect on the equilibrium vortex lattice state. Pinning shifts the resonance to higher frequencies and reduces the spectral weight of the mode, with the missing spectral weight appearing in the zero-frequency (superfluid) response (bottom right panel of Fig. 2). When $V_0' = 0$, the pinning is strongest and the resonant frequency is close to ω_{qp}. This is consistent with expectations: as the order parameter response is supressed the collective mode should increasingly resemble quasiparticle pair creation. From the Hall-angle sum rule [24,21], there is a direct relation between ω_0 and the spectral weight of the mode or, equivalently, the penetration depth:

$$\lambda^{-2} = \frac{8f_{tot}}{c^2}\left[1 - \frac{\omega_c}{\omega_0}\right], \qquad (6)$$

where the f-sum rule value, f_{tot}, is proportional to the oscillator strength of the collective mode. In Fig. 2 we show the effects of pinning on the zero-temperature penetration depth.
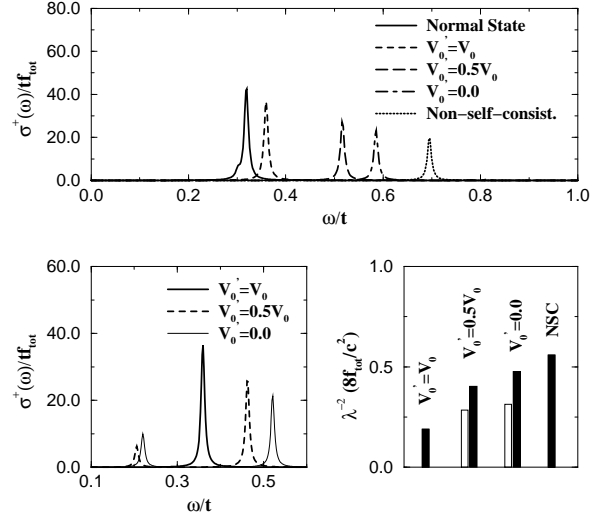
The dependence of penetration depth on pinning demonstrates the importance of distinquishing the macroscopic penetration depth of a vortex lattice, which characterizes its low frequency response to long-wavelength electromagnetic radiation, from the local effective penetration depth [25,26] measured by μSR or NMR experiments [27]. The latter is actually an equilibrium property of the vortex lattice, and an index of the inhomogeneity of the internal magnetic field distribution. (In London theory, the field distribution is determined by the zero-field penetration depth.) The μSR penetration depth is only indirectly related to the low-frequency limit of the vortex-lattice conductivity. The distinction is most stark when disorder and both extrinsic and intrinsic pinning pinning are absent; the macroscopic penetration depth should then diverge, while the local μSR penetration depth will stay close [25,26,21] to its zero-field value.

Finally, we address the case of inhomogeneous pinning, which we expect to be be typical for experimental systems and to differ importantly from the homogeneous pinning case typically studied in theoretical models [5,6]. Since our magnetic unit cells contain two vortices, we have the option of pinning them unequally. Interestingly, we find that the conductivity spectrum for the case of one pinned vortex per unit cell (bottom left panel, Fig. 2) is not congruent with the naive anticipation of independent contributions from pinned and free vortices. Instead, the collective resonance of the unpinned and homogeneously pinned cases is split, with one peak lying at $\omega < \omega_c$ and

the other at $\omega_c < \omega < \omega_{\rm qp}$. If the response were local, a peak would occur near ω_c (perhaps blue-shifted by inter-vortex forces) and a second smaller peak due to the pinned vortex would appear near $\omega_{\rm qp}$. The breakdown of the naive picture reflects the highly nonlocal nature of the clean vortex lattice response.

In summary we report on a practical numerical approach for the study of equilibrium and linear response properties in the mixed state. This work is motivated by the growing realization that high T_c superconductors are in the clean, long quasiparticle mean-free-path limit at low temperatures and by the need to avoid simplifying approximations which become dubious in this limit. In this paper we have examined the influence of pinning arrangements on the ac conductivity of dense vortex states, demonstrating the dominantly collective nature of the response and the essential role of non-locality. This type of calculation can be used to test potential paradigms and to help develop sound phenomenologies for linear response properties of these complex states.

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